Unheeded pseudo solution of Dirac-Coulomb equations with an indirect transformation of functions

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We open out one of incorrect solutions of the Driac equation in the Coulomb field given in a published paper. By introducing a transformation of function, the paper transformed the original radial first-order Dirac-Coulomb equation into two second-order Dirac-Coulomb equation. However, each of the second-order differential equations has differential energy eigenvalues set. The original paper wrote the two differential equations into one of forms, and then gave the distinguished energy eigenvalues. The mathematical procedure is not correct. For the same quantum system, introducing a transformation of function yields two different energy eigenvaluse, the result violates the uniqueness of solution. It actually shows that the given second-order differential equations have no solution. On the other hand, the given formal solutions of the second-order Dirac-Coulomb equations violate the conditions for determining solution. Consequently, the solutions given by the author are pseudo solution, and the corresponding energy eigenvalues set is also a pseudo eigenvalues set.

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I. INTRODUCTION

It is well known that, in mathematics, for a differential equation of high-order or system of differential equations of first-order, only the formal solutions satisfy the original equations, satisfy the conditions for determining solution and satisfy the uniqueness of solution or the eigensolutions set can be regard as the correct solutions. However, in relativistic quantum mechanics, it seems that many literatures are ignorant of such fundamental mathematics rules. For example, some published papers derived two different second-order Dirac-Coulomb equations for the two components of wave functions which has actually different eigenvalues sets, but finally wrote the two second-order differential equations in one form of second-order differential equations by introducing some pretexts such as so-called “decoupling procedure”[1][2], mentioning lightly, enshrouded the contradictions of violating uniqueness of solutions. In particular, those given formal solutions are not in agreement with the boundary condition. They are divergent at the origin of the coordi-

nate system. Whereas, only one use the boundary condition can determine the solution of the Draic-Coulomb equations of second order. On the other hand, in order to obtain a new energy eigenvalues, some papers even introduced the so-called position-dependent mass[3][4] to spelled backward second-order Dirac-Coulomb[5] equation, and all of the corresponding results are not the necessary mathematical deductions, including the second-order differential equations.

In the present paper, we disclose one of hidden pseudo solutions of the Dirac equations in Coulomb field, which was published in 2005. The paper first introduced a transformation of functions for the two components of wave functions, and transformed the original first-order Dirac equation in the Coulomb field into two second-order Dirac-Coulomb equations. The two second-order differential equations haave different formal eigenvalues set, violating the uniqueness of solutions, and the formal eigenfunctions are also divergent at the origin of coordinate system. But the paper wrote the two differential equations into one form, having concealed the mathematical contradiction. The paper also fenced with the boundary condition for the complete eigenfunctions. We conclude that the formula of energy-levels which corresponds to the eigenvlue set is a pseudo energy eigenvalues set for the hydrogen and hydrogen-like atom, and the given formal solutions are the pseudo solutions of the Dirac-Coulobm equations.

II. ONE OF SECOND-ORDER DIRAC-COULOMB EQUATION AND ITS PSEUDO SOLUTIONS

Discussing the single-electron or single-muon atoms for which the potential produced by the nucleus can be well approximated by a central potential $V(r)$, a paper[6] derived the coupled Dirac equations with assuming the central potential has the Coulomb form $V(r) = -Ze^2/4\pi\varepsilon_0 r$ exterior to the nucleus as follows

$$\begin{array}{c} \left(\frac{d}{dr} + \frac{1+k}{r}\right) g(r) - \frac{1}{\hbar c}\left[E + mc^2 - V(r)\right] f(r) = 0 \\ \left(\frac{d}{dr} + \frac{1-k}{r}\right) f(r) + \frac{1}{\hbar c}\left[E - mc^2 - V(r)\right] g(r) = 0 \end{array} \tag{1}$$

By introducing a mathematical transformation of functions

$$\rho = 2\sqrt{\frac{m^2c^4 - E^2}{\hbar^2 c^2}}r, \quad u = \rho^{\frac{3}{2}}\left(g - \sqrt{\frac{mc^2+E}{mc^2-E}}f\right), \quad v = \rho^{\frac{3}{2}}\left(g + \sqrt{\frac{mc^2+E}{mc^2-E}}f\right) \tag{2}$$

the system of first-order differential equations (1) with a Coulomb potential was transformed into two second-order Dirac equation for the components f and g

$$\begin{array}{c} \left\{\frac{d^2}{d\rho^2} - \frac{1}{\rho^2}\left[\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2 - \frac{1}{4}\right] + \frac{1}{\rho}\left(\frac{\alpha Z E}{\sqrt{m^2c^4 - E^2}} + \frac{1}{2}\right) - \frac{1}{4}\right\} u = 0 \\ \left\{\frac{d^2}{d\rho^2} - \frac{1}{\rho^2}\left[\left(j+\frac{1}{2}\right)^2 - (\alpha Z)^2 - \frac{1}{4}\right] + \frac{1}{\rho}\left(\frac{\alpha Z E}{\sqrt{m^2c^4 - E^2}} - \frac{1}{2}\right) - \frac{1}{4}\right\} v = 0 \end{array} \tag{3}$$

where $j = 1/2, 3/2, \cdots$, $\alpha = e^2/2\varepsilon_0 hc = e^2/4\pi\varepsilon_0\hbar c$. According to the opinion of the papers, the equations (3) have the general form of Whittaker's equation[7]

$$\left[\frac{d^2}{d\rho^2} - \frac{1}{\rho^2}\left(\gamma^2 - \frac{1}{4}\right) + \frac{\beta}{\rho} - \frac{1}{4}\right] M(\rho) = 0 \tag{4}$$

where

$$\gamma^2 = \left(j + \frac{1}{2}\right)^2 - (\alpha Z)^2, \quad \beta = \beta_\pm = \frac{\alpha Z E}{\sqrt{m^2c^4 - E^2}} \pm \frac{1}{2} \tag{5}$$

And the corresponding eigenvalues set was given as follows

$$E = mc^2 \frac{n' + \sqrt{(j+1/2)^2 - (\alpha Z)^2}}{\sqrt{(\alpha Z)^2 + \left[n' + \sqrt{(j+1/2)^2 - (\alpha Z)^2}\right]^2}}, \quad n' = 0, 1, 2, \cdots \tag{6}$$

III. EIGENVALUES SET OF EQUATIONS (3) VIOLATES UNIQUENESS OF SOLUTION

We first notice that (3) involve two different equations, but they were written in one form by introducing some new sign (5). According to the optimum theorem[8] for differential equations or the asymptotic solution and power series solution, the uncoupled equations (3) have different eigenvalues set[9]. One can demonstrate that the formula (6) for the energy levels in the Coulomb field is not a unique mathematical deduction of the system of differential equations (3). Because the original paper didn't give the detail steps of the deduction, the differential eigenvalues set for the same quantum system, meaning the obvious mathematical difficult and contradiction, are not usually taken attention to. Why don't we direct solve the second-order equations (3) without the sign (5) to find the formulas of the energy levels? The conditions for determining solution of the Dirac equations in Coulomb field are usually written in the rough form without considering the size of the atomic nucleus as same as in Schrödinger theory

$$R(r \to \infty) = 0, \quad -\infty < R(0 \le r < \infty) < \infty \tag{7}$$

Noticing the second-order differential equations (3) have the asymptotic solutions, as $\rho \to \infty$, $u \approx e^{-\frac{\rho}{2}}$ and $v \approx e^{-\frac{\rho}{2}}$ are in agreement with the boundary condition. Now we find the following form of the solution

$$u = e^{-\frac{\rho}{2}}\chi, \quad v = e^{-\frac{\rho}{2}}\sigma \tag{8}$$

We have

$$\begin{aligned}\frac{du}{d\rho} &= e^{-\frac{\rho}{2}}\left(\frac{d\chi}{d\rho}-\frac{1}{2}\chi\right), \quad \frac{d^2u}{d\rho^2} = e^{-\frac{\rho}{2}}\left(\frac{d^2\chi}{d\rho^2}-\frac{d\chi}{d\rho}+\frac{1}{4}\chi\right)\\ \frac{dv}{d\rho} &= e^{-\frac{\rho}{2}}\left(\frac{d\sigma}{d\rho}-\frac{1}{2}\sigma\right), \quad \frac{d^2v}{d\rho^2} = e^{-\frac{\rho}{2}}\left(\frac{d^2\sigma}{d\rho^2}-\frac{d\sigma}{d\rho}+\frac{1}{4}\sigma\right)\end{aligned} \tag{9}$$

Substituting (8) and (9) into the equations (3) yields

$$\begin{aligned}&\frac{d^2\chi}{d\rho^2}-\frac{d\chi}{d\rho}-\left[\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2-\frac{1}{4}\right]\frac{1}{\rho^2}\chi+\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}+\frac{1}{2}\right)\frac{1}{\rho}\chi=0\\ &\frac{d^2\sigma}{d\rho^2}-\frac{d\sigma}{d\rho}-\left[\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2-\frac{1}{4}\right]\frac{1}{\rho^2}\sigma+\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}-\frac{1}{2}\right)\frac{1}{\rho}\sigma=0\end{aligned} \tag{10}$$

For χ and σ we make the power series ansatz

$$\chi=\sum_{n=0}^{\infty}b_n\rho^{s_\chi+n}, \quad \sigma=\sum_{n=0}^{\infty}d_n\rho^{s_\sigma+n} \tag{11}$$

and insert them into the differential equations (10), giving

$$\begin{aligned}&\sum_{n=0}^{\infty}(s_\chi+n)(s_\chi+n-1)b_n\rho^{s_\chi+n-2}-\sum_{n=0}^{\infty}(s_\chi+n)b_n\rho^{s_\chi+n-1}\\ &-\left[\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2-\frac{1}{4}\right]\frac{1}{\rho^2}\sum_{n=0}^{\infty}b_n\rho^{s_\chi+n}+\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}+\frac{1}{2}\right)\frac{1}{\rho}\sum_{n=0}^{\infty}b_n\rho^{s_\chi+n}=0\\ &\sum_{n=0}^{\infty}(s_\sigma+n)(s_\sigma+n-1)d_n\rho^{s_\sigma+n-2}-\sum_{n=0}^{\infty}(s_\sigma+n)d_n\rho^{s_\sigma+n-1}\\ &-\left[\left(j+\frac{1}{2}\right)^2-(\alpha Z)^2-\frac{1}{4}\right]\frac{1}{\rho^2}\sum_{n=0}^{\infty}d_n\rho^{s_\sigma+n}+\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}-\frac{1}{2}\right)\frac{1}{\rho}\sum_{n=0}^{\infty}d_n\rho^{s_\sigma+n}=0\end{aligned} \tag{12}$$

A comparison of coefficients yields

$$\begin{aligned}&\left[(s_\chi+n)(s_\chi+n-1)-\left(j+\frac{1}{2}\right)^2+(\alpha Z)^2+\frac{1}{4}\right]b_n\\ &-\left[(s_\chi+n-1)-\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}+\frac{1}{2}\right)\right]b_{n-1}=0\\ &\left[(s_\sigma+n)(s_\sigma+n-1)-\left(j+\frac{1}{2}\right)^2+(\alpha Z)^2+\frac{1}{4}\right]d_n\\ &-\left[(s_\sigma+n-1)-\left(\frac{\alpha ZE}{\sqrt{m^2c^4-E^2}}-\frac{1}{2}\right)\right]d_{n-1}=0\end{aligned} \tag{13}$$

The above recurrence relations determine the coefficients of the power series (11). All appearance, the above relations have the initial value: $b_{-1}=d_{-1}=0$, and $b_0\neq 0$, $d_0\neq 0$. Put $n=0$ (13), we obtain

$$\begin{aligned}&\left[s_\chi(s_\chi-1)-\left(j+\frac{1}{2}\right)^2+(\alpha Z)^2+\frac{1}{4}\right]b_0=0\\ &\left[s_\sigma(s_\sigma-1)-\left(j+\frac{1}{2}\right)^2+(\alpha Z)^2+\frac{1}{4}\right]d_0=0\end{aligned} \tag{14}$$

It gives $s_\chi=s_\sigma=1/2\pm\sqrt{(j+1/2)^2-(\alpha Z)^2}$. Combining (2), (8), (11) and making use of the roots of (14) gives the complete form of the formal solutions of the original first-order Dirac equation in the Coulomb field

$$\begin{aligned}f&=\frac{1}{2}\sqrt{\frac{mc^2-E}{mc^2+E}}\rho^{-1\pm\sqrt{(j+1/2)^2-(\alpha Z)^2}}e^{-\frac{\rho}{2}}\left(\sum_{n=0}^{\infty}d_n\rho^n-\sum_{n=0}^{\infty}b_n\rho^n\right)\\ g&=\frac{1}{2}\rho^{-1\pm\sqrt{(j+1/2)^2-(\alpha Z)^2}}\left(\sum_{n=0}^{\infty}d_n\rho^n+\sum_{n=0}^{\infty}b_n\rho^n\right)\end{aligned} \tag{15}$$

Here we have replaced the original indirect transformation of functions (2) by the corresponding direct transformation of functions

$$g = \frac{1}{2}\rho^{-\frac{3}{2}}\left(v + u\right), \quad f = \frac{1}{2}\sqrt{\frac{mc^2 - E}{mc^2 + E}}\rho^{-\frac{3}{2}}\left(v - u\right) \tag{16}$$

Since the wave functions have to satisfy the boundary condition (7) at the origin of the coordinate system we must choose the positive sign for square root of index s_χ and s_σ. For the negative square root solution it follows that $f \sim \rho^{-1-\sqrt{(j+1/2)^2-(\alpha Z)^2}}$, $g \sim \rho^{-1-\sqrt{(j+1/2)^2-(\alpha Z)^2}}$ near $r = 0$ namely $\rho = 0$, which would yield a divergent integral for the norm[10]. Hence,

$$s_\chi = s_\sigma = \frac{1}{2} + \sqrt{(j + 1/2)^2 - (\alpha Z)^2} \tag{17}$$

and the formal solutions for the original Dirac-Coulomb equations(1) should be written in the form

$$\begin{array}{l} f = \frac{1}{2}\sqrt{\frac{mc^2-E}{mc^2+E}}\rho^{-1+\sqrt{(j+1/2)^2-(\alpha Z)^2}}e^{-\frac{\rho}{2}}\left(\sum\limits_{n=0}^{\infty} d_n\rho^n - \sum\limits_{n=0}^{\infty} b_n\rho^n\right) \\ g = \frac{1}{2}\rho^{-1+\sqrt{(j+1/2)^2-(\alpha Z)^2}}\left(\sum\limits_{n=0}^{\infty} d_n\rho^n + \sum\limits_{n=0}^{\infty} b_n\rho^n\right) \end{array} \tag{18}$$

On the other hand, the wave functions also have to satisfy the boundary as $r \to \infty$ namely $\rho \to \infty$ we must cut off the two power series in (18) in order to $g\left(\rho \to \infty\right) = 0$, $f\left(\rho \to \infty\right) = 0$. It is assumed that $b_{n_r} \neq 0$, $b_{n_r} \neq 0$ and $b_{n_r+1} = b_{n_r+2} = \cdots = 0$, $d_{n_r+1} = d_{n_r+2} = \cdots = 0$. Inserting $n = n_{r+1} + 1$ in the recurrence relations (13) educes that

$$\begin{array}{l} \left(\frac{1}{2} + \sqrt{(j + 1/2)^2 - (\alpha Z)^2} + n_r\right) - \left(\frac{\alpha Z E}{\sqrt{m^2c^4-E^2}} + \frac{1}{2}\right) = 0 \\ \left(\frac{1}{2} + \sqrt{(j + 1/2)^2 - (\alpha Z)^2} + n_r\right) - \left(\frac{\alpha Z E}{\sqrt{m^2c^4-E^2}} - \frac{1}{2}\right) = 0 \end{array} \tag{19}$$

It gives two positive energy eigenvalues

$$\begin{array}{l} E = \frac{mc^2}{\sqrt{1+\frac{\alpha^2 Z^2}{\left[\sqrt{(j+1/2)^2-(\alpha Z)^2}+n_r\right]^2}}} \\ E = \frac{mc^2}{\sqrt{1+\frac{\alpha^2 Z^2}{\left[\sqrt{(j+1/2)^2-(\alpha Z)^2}+n_r+1\right]^2}}} \end{array} \tag{20}$$

By all appearances, the two energy eigenvalues can not give the same set for the same quantum system in Coulomb field. Their values of energy for the ground state are not equivalent. It violates the uniqueness of solution. However, the original paper wrote the equations (10) in one of forms so as to only choose the first formula. It made a gloss that the distinguished energy eigenvalues were recovered. Such method should not be selected in any scientific paper.

IV. EIGENFUNCTIONS SET OF EQUATIONS (3) VIOLATES BOUNDARY CONDITION

Now we can write down the complete formal solutions of the first-odder Dirac equations (1) with the recurrence relations for the coefficients of the corresponding power series, in which the eigenvalues E are determined by the self-contradictory expression (3.20. Qua the formal eigenfunctions set of the original Dirac-Coulomb equations with the transformation of function (2), it is

$$\begin{array}{l} f = \frac{1}{2}\sqrt{\frac{mc^2-E}{mc^2+E}}\rho^{-1+\sqrt{(j+1/2)^2-(\alpha Z)^2}}e^{-\frac{\rho}{2}}\left(\sum\limits_{n=0}^{n_r} d_n\rho^n - \sum\limits_{n=0}^{n_r} b_n\rho^n\right) \\ g = \frac{1}{2}\rho^{-1+\sqrt{(j+1/2)^2-(\alpha Z)^2}}\left(\sum\limits_{n=0}^{n_r} d_n\rho^n + \sum\limits_{n=0}^{n_r} b_n\rho^n\right) \end{array} \tag{21}$$

When $j = 1/2$, at the origin of the coordinate system, it becomes

$$\begin{array}{l} \lim\limits_{\rho\to 0} f = \lim\limits_{\rho\to 0}\frac{1}{2}\left(d_0 - b_0\right)\sqrt{\frac{mc^2-E}{mc^2+E}}\rho^{-1+\sqrt{1-(\alpha Z)^2}}e^{-\frac{\rho}{2}} = \infty \\ \lim\limits_{\rho\to 0} g = \lim\limits_{\rho\to 0}\frac{1}{2}\left(d_0 + b_0\right)\rho^{-1+\sqrt{1-(\alpha Z)^2}} = \infty \end{array} \tag{22}$$

The formal solution for the ground state is divergent at the origin of coordinate system.

On the surface, this divergence can be explained that it has no mathematical and physical consequences, because the equations (1) have been called that it was only given outside of the atomic nucleus, and there does not exist the case $r \to 0$. However, if we accept this explain, then how to choose the positive signs for the index e_χ and e_σ in (17)? The divergence (22) implies that the probability density of the electron appearing around the atomic nucleus would rapidly increase as it near the atomic nucleus. If the formal solution (21) is the real wave function in Coulomb field, then all of the electrons would fall into the atomic nucleus. The atom would collapse to become neutron-like. It is not true! In fact, considering the atomic nucleus has a finite radius, the boundary condition would take the other form, which was called the exact boundary condition[11]. Unexpectedly, the Dirac-Coulomb equations with the exact boundary condition have different energy eigenvalues from the Dirac formula of the energy levels.

Consequently, the formal solutions (21) of the Dirac-Coulomb equation can but be understand that it violates the boundary conditions. Of course, this serious contradiction was also ignored by the original paper. In mathematics, it is well known that any formal solution which violates the condition for the determining solution must be not the real solution of the corresponding differential equation. Because of the divergence, we conclude that the necessary mathematical deductions (21) are not the real solution of the Dirac-Coulomb equation.

V. CONCLUSIONS

In a word, because the formal eigenvalues set violates the uniqueness of solution and the complete formal solutions for the ground state of the corresponding differential equations in the Coulomb field of second-order are divergent at origin, the given formula of the energy levels of the Dirac-Coulomb equation exterior to the nucleus in the mentioned paper is a pseudo energy gienvalues set, and the given wave functions, which were expressed in terms of confluent hypergeometric functions, are also the pseudo solutions of the Driac equation for the hydrogen and hydrogen-like atom. Such kind of pseudo solutions of the Dirac equations indicate that in relativistic quantum it is very important for some details being treated, such as the boundary conditions, the uniqueness of solution, the existence of eseigensolutions and the harmonic analysis and their homogenus spaces and so on[12].

For those incorrect deductions which violate the mathematical operation rules, in their papers and the quantum mechanics textbooks, some authors even called that what they related was only the physics but not mathematics, and introduced some strange words such as "mild divergence" and "decoupling procedure" and so on, which are independent of any mathematical and physical logic. However, for the quantum mechanics, once a wave equation with the certain boundary condition or initial value condition is introduced, all remnant physics should be essentially the pure mathematics. At least, anyone cannot coin some mathematic formulas for those important physics problems by using multitudinous wrong mathematics calculations. Because those hidden pseudo solutions have brought the comprehensive infection, some new correct deductions of the theoretical physics are very difficult to be known. One should disclose such kinds of pseudo theories in physics, although it is a work[13] for lollygagging. For the Dirac equation in the Coulomb field, there are many problems[14][15], in particular the localization problem and the Klein paradox[16], which need to be solved.

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